

High-pressure Diffraction Studies of Cubic ZrMo_2O_8 in a DAC

C. Lind, A. Wilkinson (Georgia Tech), J. Hriljac (U. Birmingham, UK), and T. Vogt (NSLS, Brookhaven National Lab.)

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Introduction: Negative thermal expansion (NTE) materials are of considerable scientific and technological interest. Their use in composites may facilitate the control of thermal expansion and allow the attainment of zero expansion. The high-pressure behavior of NTE materials is relevant to their application, as the NTE material will experience compression both during processing and use from the surrounding matrix material when used as a filler in a composite.

Methods and Materials: We have recently observed a phase transition to a new high-pressure polymorph in the NTE material cubic ZrMo_2O_8 at pressures between 0.7 and 1.5 GPa. This reversible first order transition, which decreases the unit cell volume by $\sim 11\%$, seems to involve a lowering of the lattice symmetry. However, the data collected with monochromatic radiation in a multi anvil press did not allow us to determine the symmetry of the new phase. To address this issue, we performed experiments in a diamond anvil cell (DAC) in the hope of better resolution. Two sets of experiments were carried out, one with a MeOH/EtOH/ H_2O (16:3:1) mixture as pressure transmitting medium and one with fluorinert.

Results: The data collected in the alcohol mixture does not show any peak splitting even at 3.14 GPa. The extracted lattice constants are systematically larger than our values obtained from the multi anvil press experiments, while the values from the DAC run in fluorinert agree with the multi anvil data. The only run in fluorinert above the transition pressure (3.03 GPa) demonstrates the lowering of the lattice symmetry by revealing some peak splitting. However, the resolution of the data was still not good enough for an unambiguous determination of the lattice symmetry.